

Tunnel splittings for one dimensional potential wells revisited

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Abstract

The WKB and instanton answers for the tunnel splitting of the ground state in a symmetric double well potential are both reduced to an expression involving only the functionals of the potential, without the need for solving any auxilliary problems. This formula is applied to simple model problems. The prefactor for the splitting in the text book by Landau and Lifshitz is amended so as to apply to the ground and low lying excited states.

I. INTRODUCTION

The purpose of this article is to reexamine some formal aspects of the problem of calculating the quantum mechanical tunnel splittings in a smooth, symmetric, one-dimensional double well potential, such as that in Fig. 1. Readers may justifiably wonder if anything new remains to be said on so mature a subject, and we assure them that, by and large, there isn't. The physical phenomenon is certainly very well understood, as are the basic mathematical ideas behind the calculations. We find, nevertheless, that especially in the case of the ground state splitting, there is some confusion regarding the correct WKB answer for this splitting, which is often taken in a form that is less accurate than it needs to be. In particular, we note that the formula for the splitting in the masterly text book by Landau and Lifshitz [1] leads to a prefactor which is incorrect for the ground state [2]. A second problem is that the form in which this result is usually presented is poorly suited to calculation of the ground state splitting. In applying it to model problems such as the quartic double well potential, e.g., the unwary student is unnecessarily led into asymptotic expansions of elliptic integrals, which must then be taken from standard tables of formulas. Because of this confusion, there is also confusion regarding the equivalence of the WKB [1] and the instanton [3,4] methods for calculating tunnel splittings.

Like many other problems in physics of a similar nature, the above discrepancies and their resolution are at the same time “well-known” and not known at all! They are well-known to some experts. Thus, the correct answers for the splitting are implicit throughout early WKB studies of the anharmonic oscillator [5,6], and can be ferreted out with some work. They are also clearly known to many field theorists [4–10], and to authors of more pedagogical articles [11,12]. At the same time, the confusion persists, and continues to crop up from time to time. Thus it seems worthwhile to address this issue here.

It should also be stated at the outset that our article is of no interest if one only wants the splitting to “exponential accuracy”, i.e., if one only wants the Gamow factor. In most physical applications, this is all that can sensibly be done, and the prefactor is best estimated as an “attempt frequency.” From a mathematical point of view, however, the tunnel splitting is found as an asymptotic approximation in the limit $\hbar \rightarrow 0$. An “exponentially accurate” answer for the splitting Δ is one for which one only has an asymptotically correct result for $\ln \Delta$. An asymptotically correct answer for Δ itself requires worrying about the prefactor. More importantly, any formalism which did not give this prefactor, or which was incapable of giving it correctly even in principle, would be regarded as logically unsound. It is from this perspective that the prefactor is important. The confusion that is referred to above can be said to pertain solely to this prefactor, and readers who are not concerned with such arcana should stop reading here. On the other hand, the WKB analysis presented here is easily incorporated into a graduate level discussion of tunnel splittings, with little additional effort beyond that of the standard treatment, and there is no reason not to do so. The problem may also serve as a “real-life” physics example of some nontrivial asymptotic analysis. (To avoid misunderstanding, let us also state at the outset what we mean by WKB theory. We use the term in the broad sense used by Bender and Orszag [13], or by Berry and Mount [14], i.e., as a body of mathematical techniques that yield global understanding and systematic asymptotic approximations to solutions of many linear differential equations,

FIGURES

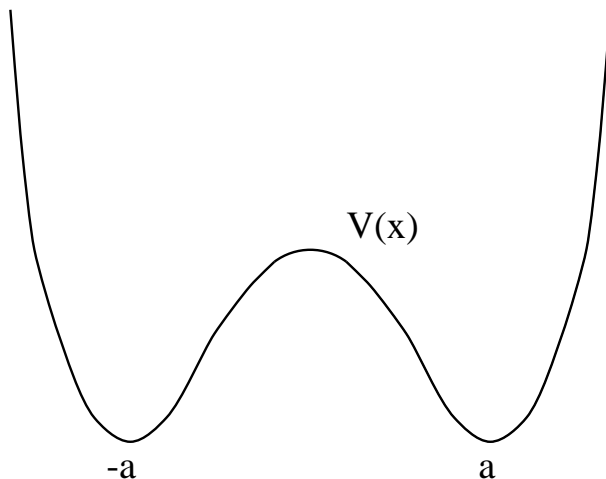


FIG. 1. Symmetric double well potential $V(x)$ considered in this paper. The minima at $x = \pm a$ are taken to be quadratic.

including Schrödinger's equation, and shares ideas with other methods such as asymptotic matching and patching, boundary layer theory, etc. Some readers may, however, define WKB to encompass only the approximate exponential form (2.2) (and its oscillatory counterpart) and connection formulas at linear turning points. A subset of these readers may recognize that our treatment in Sec. II is tantamount to the use of quadratic turning point [15] connection formulas (for which see Berry and Mount [14]), and object that this goes beyond WKB. Such a semantic restriction of the scope of the term 'WKB', should in our view, be avoided. Since the method did not originate with Wentzel, Kramers, and Brillouin, but had antecedents in the work of Jeffreys, Rayleigh, Carlini, Green, Liouville, and perhaps others, there is no compelling historical reason for this restriction (as opposed to say, the usages 'Einstein model' for lattice specific heat, or the 'Kronig-Penney model' for electrons in a periodic potential), and it is surely more useful to present the subject to students as one which allows for systematic improvement, and is not a closed subject of study even today.)

It is with this motivation that we revisit the problem of calculating tunnel splittings in symmetric double well potentials. The article has three distinct aims. The first is to carefully calculate the prefactor multiplying the exponential of the turning-point-to-turning-point action integral in the standard WKB expression for the splitting Δ . The correct formula is Eq. (1.1) below. Our second aim is to present another formula [See Eqs. (1.4–1.6)] for the ground state splitting [16], that reduces everything to the evaluation of two integrals involving the potential $V(x)$, and does not require looking up any asymptotic expansions. The last aim is to show that the correct WKB and instanton [3,4] methods do yield the same ground state splitting. We will do this by starting with Coleman's instanton method expression for the splitting [4] and showing that it reduces to our simple formula.

We expect that our WKB based discussion will be accessible to students who have seen some graduate level quantum mechanics, even though our starting formula for the splitting is rarely ever mentioned in the common text books. One book where it does appear is again that of Landau and Lifshitz [1], who give an exceptionally lucid and self-contained discussion. We will comment further on this formula when we come to it in Sec. II, and give

a separate derivation of it in Appendix A. The instanton formalism, and the path integral approach to quantum mechanics upon which it is in turn based, are less likely to be familiar, but clear and accessible discussions have been given in this journal by Holstein [11], and by Holstein and Swift [12]. The former discusses exactly the same problem as us, namely, the tunnel splitting, but for the special case of a quartic double well. We enthusiastically recommend Coleman's somewhat longer but authoritative article on instantons [4] to readers who wish to learn more about this technique. A related paper by Carlitz and Nicole [17] may also be read profitably.

A plan of our paper and summary of our results is as follows. We consider a potential which is smooth, reflection symmetric about $x=0$ [$V(-x) = V(x)$], and which has quadratic minima at $x = \pm a$. The correct WKB answer for the ground state splitting is [18]

$$\Delta = \frac{\hbar\omega}{\sqrt{e\pi}} \exp\left[-\int_{-a'}^{a'} \frac{|p|}{\hbar} dx\right]. \quad (1.1)$$

Here, ω is the frequency of small amplitude oscillations in the wells about $x = \pm a$, $\pm a'$ are the classical turning points given by the equation

$$V(a') = E_0 = \frac{1}{2}\hbar\omega + o(\hbar), \quad (1.2)$$

and p is the momentum

$$p(x) = [2m(V(x) - E)]^{1/2}. \quad (1.3)$$

Note that $p(x)$ is imaginary in the classically forbidden region $-a' < x < a'$, and that we have taken $V(\pm a) = 0$.

The proof of Eq. (1.1) is given in Sec. II. This entails matching the WKB wavefunction in the classically forbidden region to the exact harmonic oscillator wavefunction near the classical turning point, rather than use the connection formulas. This matching calculation may actually be found in a paper by Furry [19], but we include it because it is very short, and so as to have the complete argument in one place in a consistent notation.

Prefactor corrections similar to those in Eq. (1.1) accompany the excited states too, and are discussed in Appendix B.

The expression (1.1) is not easy to use because the integrand in the exponential is close to a singularity near the limits, which means that the next to leading dependence of Δ on \hbar is not manifest. In fact, the true preexponential factor varies as $\hbar^{1/2}$, and this is not obvious from Eq. (1.1). In Sec. III, we shall, therefore, carefully extract the singular contributions to the action integral from the end points, and show that the splitting may be written for a general potential as

$$\Delta = 2\hbar\omega \left(\frac{m\omega a^2}{\pi\hbar}\right)^{1/2} e^A e^{-S_0/\hbar}, \quad (1.4)$$

where S_0 (note the limits of integration) is the action integral

$$S_0 = \int_{-a}^a (2mV(x))^{1/2} dx, \quad (1.5)$$

and

$$A = \int_0^a \left[\frac{m\omega}{\sqrt{2mV(x)}} - \frac{1}{a-x} \right] dx. \quad (1.6)$$

This expression does not have the complexities mentioned above. The $\hbar^{1/2}$ dependence of the prefactor is apparent, and the answer involves only integral functionals of $V(x)$. These formulas will be applied to two model problems in Sec. V.

In Sec. IV, we turn to the instanton approach [3,4]. Here, the splitting is expressed as

$$\Delta = 2\hbar K \left(\frac{S_0}{2\pi\hbar} \right)^{1/2} \exp(-S_0/\hbar), \quad (1.7)$$

where S_0 is as in Eq. (1.5), and

$$K = \left[\frac{\det(-\partial_\tau^2 + \omega^2)}{\det'[-\partial_\tau^2 + m^{-1}V''(x_{\text{cl}}(\tau))]} \right]^{1/2} \quad (1.8)$$

is the ratio of fluctuation determinants. Here, $x_{\text{cl}}(\tau)$ is the instanton, which obeys the (Euclidean) classical equation of motion

$$m \frac{d^2 x_{\text{cl}}(\tau)}{d\tau^2} - V'(x_{\text{cl}}) = 0, \quad (1.9)$$

with the boundary conditions $x_{\text{cl}}(\pm\infty) = \pm a$, and the additional condition $x_{\text{cl}}(0) = 0$ to fix the time translation degree of freedom. Further, $V' = dV/dx$, $V'' = d^2V/dx^2$, and the prime on the det in Eq. (1.8) means that the zero eigenvalue of the operator argument is to be excluded from a product of all eigenvalues.

A short and pedagogical discussion of the instanton method may be found in Holstein [11]. Holstein does not explain how to calculate the quantity K (which is proportional to his quantity K_1), so a few remarks that help elucidate its nature may not be out of place. Note first, that each determinant appearing in Eq. (1.8) is of a one-dimensional Schrodinger-like operator, in which τ plays the role of position, and either ω^2 or $m^{-1}V''(x_{\text{cl}}(\tau))$ plays the role of the potential energy. Next we note, that the determinant of such an operator may be defined as an infinite product of all its eigenvalues. The spectrum of operators at hand may be rendered completely discrete by adding hard walls at $\tau = \pm T$, and letting $T \rightarrow \infty$ at the end. This scheme has the advantage that it allows us to put the eigenvalues of both operators in one-to-one correspondence. This in turn enables us to argue that one eigenvalue is missing in the denominator, and since the eigenvalues have the dimensions of ∂_τ^2 or ω^2 , we see that K has the dimensions of frequency. For a smooth potential $V(x)$, the curvature $m^{-1}V''(x_{\text{cl}}(\tau))$ is never very different from ω^2 in the interval $-a \leq x \leq a$, so there is only one frequency scale in the problem. It follows that K is of order ω .

To the author's knowledge, the equivalence of Eqs. (1.1) and (1.7) has only been shown for particular examples, such as the quartic double well potential. A general demonstration is lacking, although it is implicit in the fact that both methods start from the same point and are correctly executed. A direct demonstration is therefore of some value. Secondly, Eq. (1.7) is complicated just as Eq. (1.1) was. Indeed, the ratio of determinants seems

more intimidating and harder to calculate than the integral in Eq. (1.1). Langer's original calculation [3] for K is quite involved, and while it has been greatly simplified by Coleman [4], it still requires solving the auxilliary problem of finding the instanton $x_{\text{cl}}(\tau)$.

To relate the instanton and WKB answers, we therefore show in Sec. IV, that Coleman's result for K may be expressed in terms of the integral A in Eq. (1.6). Thus, although we do not provide a complete derivation of the instanton result for Δ , once Coleman's formulas are accepted, our analysis shows the equivalence of the two approaches.

II. WKB FORMULA FOR GROUND STATE SPLITTING

Our starting point is the formula [20]

$$\Delta = \frac{2\hbar^2}{m}\psi_0(0)\psi'_0(0), \quad (2.1)$$

where $\psi_0(x)$ is an approximate solution to Schrödinger's equation with energy E_0 , which is localized in the right hand well, and decays away from that well, in the *entire* central, classically forbidden region. Further, it is normalized to yield unit total probability in the right hand well. Note that it is not necessary to examine or specify the behaviour of $\psi_0(x)$ near $x = -a'$. Lastly, $\psi'_0(x) = d\psi_0(x)/dx$.

We digress briefly at this point to comment on the formula (2.1), which does not seem to be widely known. It is sometimes named after Conyers Herring, who derived it (in a slightly more general form, in fact) in the course of evaluating the g - u splitting of the two lowest electronic states of the H_2^+ molecular ion [21,22]. The actual derivation is simple, and very similar to the usual half-page of analysis used to argue that the the Hamiltonian operator in the position representation is Hermitean and has real eigenvalues, and so we refer readers to Landau and Lifshitz [1] for the details. Instead, we present an alternative derivation in Appendix A.

Resuming our argument, we note that the WKB approximation for $\psi_0(x)$ in the region $(a' - x) \gg (\hbar/m\omega)^{1/2}$ is

$$\psi_0(x) = \frac{C_0}{\sqrt{|v(x)|}} \exp \frac{1}{\hbar} \int_0^x |p(x')| dx', \quad (2.2)$$

where $v(x) = p(x)/m$, and C_0 is a constant to be found by matching on to the solution in the well. To the accuracy of this solution, $\psi'_0(x) \approx (m|v(x)|/\hbar)\psi_0(x)$, so that

$$\Delta = 2\hbar C_0^2. \quad (2.3)$$

To find C_0 , we first note that near $x = a$, $\psi_0(x)$ is very accurately given by the ground state harmonic oscillator wave function

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp \left[-\frac{m\omega}{2\hbar}(x - a)^2\right]. \quad (2.4)$$

In fact, this form holds well into the forbidden region, and so can be directly matched to Eq. (2.2) without invoking connection formulas. In the overlap region, we may write

$$|p(x)| = m\omega \left[(a-x)^2 - u_0^2 \right]^{1/2}, \quad (2.5)$$

where

$$u_0 = a - a' \approx (\hbar/m\omega)^{1/2}. \quad (2.6)$$

The term u_0^2 in Eq. (2.5) may be neglected in evaluating the $|v(x)|^{-1/2}$ prefactor in Eq. (2.2), so that we may write

$$\psi_0(x) \approx \frac{C_0}{\sqrt{\omega(a-x)}} \exp \left[\frac{1}{\hbar} \int_0^{a'} |p(x')| dx' + \Phi(x) \right], \quad (2.7)$$

where

$$\begin{aligned} \Phi(x) &= -\frac{m\omega}{\hbar} \int_x^{a'} \left[(a-x')^2 - u_0^2 \right]^{1/2} dx' \\ &\approx -\frac{m\omega(a-x)^2}{2\hbar} + \ln \left(\frac{2(a-x)}{u_0} \right)^{1/2} + \frac{1}{4} + O \left(\frac{u_0}{a-x} \right)^2. \end{aligned} \quad (2.8)$$

Comparing Eqs. (2.7) and (2.8) with Eq. (2.4), we obtain

$$C_0 = \left(\frac{\omega^2}{4\pi e} \right)^{1/4} \exp \left[-\frac{1}{\hbar} \int_0^{a'} |p(x)| dx \right]. \quad (2.9)$$

Substituting Eq. (2.9) in Eq. (2.3), and making use of the reflection symmetry of $V(x)$, we obtain

$$\Delta = \frac{\hbar\omega}{\sqrt{e\pi}} \exp \left[-\int_{-a'}^{a'} \frac{|p|}{\hbar} dx \right], \quad (2.10)$$

which is Eq. (1.1).

Landau and Lifshitz obtain C_0 by using connection formulas near a linear turning point, and the standard WKB result for the normalization of a bound state. For the ground state, this procedure is not accurate enough, and we must proceed as above. (Some readers may recognize in our procedure, the use of quadratic turning point formulas [14].) Once this is realized, similar prefactor corrections are expected for the low lying excited states. These corrections are obtained in Appendix B.

III. SIMPLER EXPRESSION FOR GROUND STATE SPLITTING

In this section we will show that the WKB expression (1.1) leads to the simpler result (1.4–1.6). The objective, clearly, is to let the action integral run from $-a$ to a instead of from $-a'$ to a' . To that end, let us denote $y = a - x$, $V(x) = U(y)$, and define, for a general u ,

$$I(u) = \int_u^a [2m(U(y) - U(u))]^{1/2} dy. \quad (3.1)$$

The quantity $I(u_0)$ is clearly half the action integral in Eq. (1.1), i.e.,

$$I(u_0) = \frac{1}{2\hbar} \int_{-a'}^{a'} |p(x)| dx. \quad (3.2)$$

Our goal is to expand $I(u)$ for small u . The analysis in Sec. II reveals [see Eq. (2.8)] that this expansion contains a term varying as $u^2 \ln u$, which means that the expansion cannot be found by simply differentiating $I(u)$. More precisely, the term of order $u^2 \ln u$ is easily found, but the term of order u^2 , which we also need, is rather harder to get.

We therefore resort to a subtraction and write $I(u) = I_1(u) + I'_1(u)$, where

$$I_1(u) = \int_u^a \sqrt{2mU(y)} dy, \quad (3.3)$$

$$I'_1(u) = \int_u^a \left(\sqrt{2m[U(y) - U(u)]} - \sqrt{2mU(y)} \right) dy. \quad (3.4)$$

$I_1(u)$ can be directly expanded:

$$\begin{aligned} I_1(u) &\approx \int_0^a \sqrt{2mU(y)} dy - \int_0^u \left(m\omega y + O(y^2) \right) dy \\ &= I(0) - \frac{1}{2} m\omega u^2 + O(u^3), \end{aligned} \quad (3.5)$$

while for $I'_1(u)$ we have, as $u \rightarrow 0$,

$$I'_1(u) \approx -(m\omega u)^2 \int_u^a \frac{dy}{\sqrt{2m[U(y) - U(u)]} + \sqrt{2mU(y)}}. \quad (3.6)$$

Note that in writing this expression, we have taken $U(u) \approx m\omega^2 u^2/2$ in the numerator, as u is small. It still can not be expanded directly, however, so we perform another subtraction, and write $I'_1 = I_2 + I_3$, where

$$I_2(u) = -\frac{1}{2} (m\omega u)^2 \int_u^a \frac{dy}{\sqrt{2m[U(y) - U(u)]}}. \quad (3.7)$$

The difference I_3 contains a proportionality factor $U(u)$, which we again approximate by $m\omega^2 u^2/2$. This leads to

$$I_3(u) \approx -\frac{1}{2} (m\omega u)^4 \int_u^a \frac{dy}{\sqrt{2m[U(y) - U(u)]} \left[\sqrt{2m[U(y) - U(u)]} + \sqrt{2mU(y)} \right]^2}. \quad (3.8)$$

Let us consider $I_2(u)$ first. We can clearly write the integral as

$$\int_u^a \frac{dy}{m\omega \sqrt{y^2 - u^2}} + \int_u^a \left[\frac{1}{\sqrt{2m[U(y) - U(u)]}} - \frac{1}{m\omega \sqrt{y^2 - u^2}} \right] dy. \quad (3.9)$$

The first integral can be done exactly, while in the second we can set $u = 0$ inside the integrand and in the limits to leading order. We thus find

$$I_2(u) \approx -\frac{1}{2}m\omega u^2 \ln \frac{2a}{u} - \frac{1}{2}(m\omega u)^2 \int_0^a \left[\frac{1}{\sqrt{2mU(y)}} - \frac{1}{m\omega y} \right] dy + O(u^4 \ln u). \quad (3.10)$$

The leading behaviour of $I_3(u)$, on the other hand, is controlled by the lower limit in the integral (3.8), where we can again approximate $U(y)$ by $m\omega^2 y^2/2$. Hence,

$$\begin{aligned} I_3(u) &\approx \frac{1}{2}m\omega u^4 \int_u^a \frac{dy}{\sqrt{y^2 - u^2} [\sqrt{y^2 - u^2} + y]^2} \\ &\approx \frac{1}{4}m\omega u^2 + O(u^4). \end{aligned} \quad (3.11)$$

Collecting together Eqs. (3.5), (3.10), and (3.11), and putting $u = u_0 = (\hbar/m\omega)^{1/2}$, we get

$$I(u_0) \approx I(0) - \frac{\hbar}{2} \ln \frac{2a}{u_0} - \frac{\hbar}{4} - \frac{\hbar}{2} \int_0^a \left[\frac{m\omega}{\sqrt{2mU(y)}} - \frac{1}{y} \right] dy + \dots \quad (3.12)$$

The last integral in the above equation is nothing but the quantity A defined in Eq. (1.6). Using $u_0 = (\hbar/m\omega)^{1/2}$ once again, and putting together Eqs. (3.12), (3.2), and (1.1), we get

$$\Delta = \frac{2\hbar\omega}{\sqrt{e\pi}} \left(\frac{m\omega a^2}{\hbar} \right)^{1/2} \sqrt{e} e^A e^{-2I(0)/\hbar}. \quad (3.13)$$

Since $I(0) = S_0/2$, this is nothing but Eq. (1.4).

IV. EQUIVALENCE OF WKB AND INSTANTON RESULTS

Our next step is to show that the instanton result (1.7) also leads to Eqs. (1.4–1.6), and thus prove the equivalence of the WKB and instanton results for the ground state splitting. To do this, we use Coleman's result for the ratio K [4]. According to him,

$$K = \sqrt{2\omega}\beta, \quad (4.1)$$

where β is related to the asymptotic, $\tau \rightarrow \pm\infty$ behaviour of the instanton velocity via

$$x_1(\tau) \equiv \left(\frac{m}{S_0} \right)^{1/2} \frac{dx_{\text{cl}}}{d\tau} \approx \beta e^{\mp\omega\tau} \quad \text{as } \tau \rightarrow \pm\infty. \quad (4.2)$$

It is easy to integrate the equation of motion (1.9) for the instanton, and obtain $x_1(\tau)$. Using the fact that $x_{\text{cl}}(0) = 0$, we have

$$\tau = m \int_0^{x_{\text{cl}}} \frac{dx}{\sqrt{2mV(x)}}. \quad (4.3)$$

This diverges as $x_{\text{cl}} \rightarrow a$, as it should. We extract the divergence by subtracting and adding the leading singular part of the integrand. This yields,

$$\begin{aligned}\tau &= m \int_0^{x_{\text{cl}}} \left[\frac{1}{\sqrt{2mV(x)}} - \frac{1}{m\omega(a-x)} \right] dx + \frac{1}{\omega} \ln \left(\frac{a}{a-x_{\text{cl}}} \right) \\ &\approx \frac{1}{\omega} \ln \left(\frac{a}{a-x_{\text{cl}}} \right) + \frac{A}{\omega} \quad \text{as } x_{\text{cl}} \rightarrow a.\end{aligned}\tag{4.4}$$

A is, of course, the quantity defined in Eq. (1.6).

Thus, as $\tau \rightarrow \infty$,

$$x_{\text{cl}}(\tau) \approx a - ae^A e^{-\omega\tau},\tag{4.5}$$

$$\frac{dx_{\text{cl}}}{d\tau} \approx a\omega e^A e^{-\omega\tau}.\tag{4.6}$$

Comparing with Eq. (4.2), we can read off β immediately:

$$\beta = a\omega \left(\frac{m}{S_0} \right)^{1/2} e^A.\tag{4.7}$$

Hence,

$$K = a\omega \left(\frac{2m\omega}{S_0} \right)^{1/2} e^A,\tag{4.8}$$

and

$$\Delta = 2\hbar\omega \left(\frac{m\omega a^2}{\pi\hbar} \right)^{1/2} e^A e^{-S_0/\hbar},\tag{4.9}$$

which is what we set out to show.

V. ILLUSTRATIVE EXAMPLES

We conclude with two elementary examples to which we apply Eqs. (1.4–1.6).

The first example is that of the quartic double well,

$$V(x) = V_0(x^2 - a^2)^2/a^4.\tag{5.1}$$

Here, V_0 is the barrier height. The frequency ω is given by

$$\omega = (8V_0/ma^2)^{1/2}.\tag{5.2}$$

It is simple to perform the integrals, and show that

$$\frac{S_0}{\hbar} = \frac{4}{3} \left(\frac{2mV_0a^2}{\hbar^2} \right)^{1/2} = \frac{16}{3} \frac{V_0}{\hbar\omega},\tag{5.3}$$

$$A = \ln 2.\tag{5.4}$$

Further, $(m\omega a^2/\pi\hbar)^{1/2} = (3S_0/2\pi\hbar)^{1/2}$, so that

$$\Delta = 4\sqrt{3}\hbar\omega \left(\frac{S_0}{2\pi\hbar}\right)^{1/2} e^{-S_0/\hbar}, \quad (5.5)$$

which is a well known form for the answer.

Our second example involves the spin Hamiltonian

$$\mathcal{H} = -\gamma S_z^2 - \alpha S_x, \quad (5.6)$$

where S_α ($\alpha = x, y, z$) are components of the dimensionless spin operator \mathbf{S} obeying the commutation rules $[S_\alpha, S_\beta] = i\epsilon_{\alpha\beta\gamma}S_\gamma$, and we also take $\alpha > 0$, $\gamma > 0$.

In the limit where the magnitude S of the spin is very large [23], Eq. (5.6) can be viewed as tending to a classical Hamiltonian, wherein the dynamics are defined by giving the Poisson brackets $[S_\alpha, S_\beta]_{\text{PB}} = \epsilon_{\alpha\beta\gamma}S_\gamma$. The classical energy has two degenerate minima when the spin lies in the xz plane at angles θ_0 or $\pi - \theta_0$ to the z axis, where

$$\sin \theta_0 = \alpha/2\gamma S. \quad (5.7)$$

For the quantum mechanical problem, with large but finite S , we expect the ground states around these classical orientations to be admixed by tunneling, thus giving rise to a small splitting of the energy levels.

Compared to the tunneling of massive particles with a position coordinate, the tunneling of spins is somewhat less familiar, but it is a perfectly bona fide instance of the general tunneling phenomenon. Spin tunnel splittings have been calculated by a variety of means for some time now [24,25], but obtaining the prefactors in the tunnel splittings correctly to order S^0 as $S \rightarrow \infty$, has proven to be a fairly difficult task, and the instanton calculations [24,26] are especially subtle. The discrete WKB method uses only elementary methods of analysis, but the calculations to date [25,27] are still lengthy. There is an even simpler method, however, which is due to Scharf, Wreszinski, and van Hemmen [28]. These authors expand a general state $|\psi\rangle$ in the S_z eigenbasis $\{|m\rangle\}$ ($S_z|m\rangle = m|m\rangle$) as $|\psi\rangle = \sum_m D_m|m\rangle$, and construct a generating function $\sum_m D_m x^m$. After a few changes of variables, the Schrödinger equation for $|\psi\rangle$ is turned into the following Schrödinger equation [See their Eq. (2.17)] for a wavefunction $y(z)$ related to the generating function:

$$-\gamma^2 \frac{d^2 y}{dz^2} + V(z)y(z) = \gamma E y(z), \quad (5.8)$$

with the potential

$$V(z) = \frac{1}{4}\alpha^2(\cosh z - \cosh z_0)^2, \quad (5.9)$$

$$\cosh z_0 = (2S + 1)\gamma/\alpha. \quad (5.10)$$

The quantity E in Eq. (5.8) is the energy eigenvalue of the Hamiltonian (5.6).

The potential (5.9) is even about $z = 0$, and has minima at $\pm z_0$. Our formalism is directly applicable if we identify $\hbar^2/2m$ with γ^2 , and $m\omega^2$ with $V''(\pm z_0) = \frac{1}{2}\alpha^2 \sinh^2 z_0$. The action integral (1.5) is easily seen to be

$$\begin{aligned} \frac{S_0}{\hbar} &= \frac{\alpha}{\gamma} \int_0^{z_0} (\cosh z_0 - \cosh z) dz \\ &= \frac{\alpha}{\gamma} (z_0 \cosh z_0 - \sinh z_0), \end{aligned} \quad (5.11)$$

while the correction (1.6) is given by

$$A = \int_0^{z_0} \left[\frac{\sinh z_0}{\cosh z_0 - \cosh z} - \frac{1}{z_0 - z} \right] dz. \quad (5.12)$$

Since the integrand is nonsingular at $z = z_0$ (or if one so wishes to view matters, has a removable singularity at that point), the integral can be found by changing the upper limit to $z_0 - \delta$, integrating the two terms separately, and letting $\delta \rightarrow 0$ at the end. The integrals involved are elementary, and the final result is

$$A = \ln \left(\frac{2 \sinh z_0}{z_0} \right). \quad (5.13)$$

It remains to substitute Eqs. (5.11) and (5.13) into our general formula (1.4). Recalling the factor of γ on the right hand side of Eq. (5.8), and the equivalences $\hbar^2/2m \equiv \gamma^2$, $m\omega^2 \equiv V''(z_0)$, we obtain

$$\Delta = \frac{4\alpha^{3/2} \sinh^{5/2} z_0}{\sqrt{2\pi\gamma}} \exp \left[-\frac{\alpha}{\gamma} (z_0 \cosh z_0 - \sinh z_0) \right]. \quad (5.14)$$

It is easier to interpret this result if it is cast in terms of the angle θ_0 in Eq. (5.7). After a certain amount of tedious algebra, one obtains, correct to order S^0 as $S \rightarrow \infty$,

$$\Delta = \frac{8\gamma S^{3/2} \cos^{5/2} \theta_0}{\pi^{1/2} \sin \theta_0} \left(\frac{1 - \cos \theta_0}{1 + \cos \theta_0} \right)^{S+1/2} e^{2S \cos \theta_0}. \quad (5.15)$$

This is precisely the form quoted in Ref. [27]. Its relation to previous calculations is discussed there.

From the viewpoint of this article, the interesting comparison is with Scharf, Wreszinski, and van Hemmen [28]. These authors only consider the case where α and γ are fixed as $S \rightarrow \infty$, so that $\theta_0 = O(1/S)$. In that limit, they follow the Landau-Lifshitz prescription, and obtain a ground state splitting $\Delta' = (2S/\pi)e^J$, with

$$J = -2S \ln \left(\frac{8}{\alpha} \gamma^2 S^2 \right) + 2S + (2S + 1) \ln \left[\gamma(2S + \tfrac{1}{2}) \right] - \frac{1}{2} \ln \left[\gamma^2(S + \tfrac{1}{4}) \right]. \quad (5.16)$$

With a little work one can show that Δ'/Δ is exactly $(e/\pi)^{1/2}$. The discrepancy can in fact be seen in the comparison between numerical and analytical results in Table 1 of Ref. [28]. While $(e/\pi)^{1/2} = 0.930$, the ratio of their analytical answer for the splitting to the numerical one (see the last two columns) decreases from 0.987 to 0.951 as S increases from 5 to 11, which is quite close. A Richardson transformation [29] of this ratio does suggest that it tending to 0.93, but one cannot be certain of this conclusion, as there are two erratic values at 0.90 and 0.91.

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APPENDIX A: HERRING'S FORMULA

Let us denote the two states localized in the left and right wells by $|R\rangle$ and $|L\rangle$ respectively. These states are degenerate in the absence of tunneling with an energy E_0 . The tunnel splitting is Δ . The Hamiltonian matrix in this two-state subspace is given by

$$\mathcal{H} = \begin{pmatrix} E_0 & \Delta/2 \\ \Delta/2 & E_0 \end{pmatrix} \quad (\text{A1})$$

Assuming that the system starts in the state $|R\rangle$ at $t = 0$, it is straightforward to show that the probability $P_R(t)$ for finding it in the same state at a later time t is given by

$$P_R(t) = \cos^2(\Delta t/2\hbar). \quad (\text{A2})$$

In particular,

$$\frac{dP_R}{dt} = -\frac{\Delta}{2\hbar} \sin\left(\frac{\Delta t}{\hbar}\right). \quad (\text{A3})$$

To relate this abstract space description to that in position space, we make use of the continuity equation for probability. For a general wave function $\psi(x, t)$ that obeys Schrödinger's equation, the probability density $P(x, t) = |\psi(x, t)|^2$ obeys

$$\frac{\partial P(x, t)}{\partial t} = -\frac{\hbar}{m} \frac{\partial}{\partial x} \text{Im}[\psi^*(x, t)\psi'(x, t)], \quad (\text{A4})$$

where $\psi' \equiv \partial\psi/\partial x$. The probability $P_R(t)$ for being in the right well is then given by

$$P_R(t) = \int_0^\infty P(x, t) dx. \quad (\text{A5})$$

Differentiating with respect to t , making use of the continuity equation, and the fact that $\psi(x, t) \rightarrow 0$ as $x \rightarrow \infty$ for any well behaved solution, we obtain

$$\frac{dP_R(t)}{dt} = \frac{-\hbar}{m} \text{Im}[\psi^*(0, t)\psi'(0, t)]. \quad (\text{A6})$$

Let us finally consider the states $|R\rangle$ and $|L\rangle$ in position space. It is evident that we should take $\langle x|R\rangle$ to be the function described as $\psi_0(x)$ in Sec. II. By symmetry, $\langle x|L\rangle = \psi_0(-x)$, and the energy eigenstates are $(\psi_0(x) \pm \psi_0(-x))/\sqrt{2}$. It then follows that with the same initial conditions as above, the wave function at an arbitrary time t is given by

$$\psi(x, t) = \psi_0(x) \cos(\Delta t/2\hbar) + i\psi_0(-x) \sin(\Delta t/2\hbar). \quad (\text{A7})$$

Hence,

$$\text{Im}[\psi^*(0, t)\psi'(0, t)] = \psi_0(0)\psi'_0(0) \sin(\Delta t/\hbar). \quad (\text{A8})$$

Substituting this result in Eq. (A6) and comparing with Eq. (A3), we obtain

$$\Delta = (2\hbar^2/m)\psi_0(0)\psi'_0(0), \quad (\text{A9})$$

which is Eq. (2.1), Herring's formula.

It is apparent from our derivation that Herring's formula holds whenever the energy eigenfunctions are well approximated by the combinations $(\psi_0(x) \pm \psi_0(-x))/\sqrt{2}$. (More precise statements of the conditions for its validity are given in Ref. [21].) Use of this formula greatly simplifies the labour required to solve all the standard double-well problems: the double square well with infinite side walls [30,31], the double delta function [31], and the double harmonic oscillator with a kink [32]. For smooth potentials, where WKB is indicated, it is far superior to the approach where one uses connection formulas at all four turning points [33]. Further, the formula brings out the physical point that a tunnel *splitting* is intimately related to a tunneling *amplitude*, since it relates the amplitude to make a transition between wells per unit time, $-i\Delta/\hbar$, to the probability current.

The reader will also have noticed that the above argument cannot be carried out for an asymmetric potential, and indeed the very concept of tunnel splitting is then very delicate. A tunneling amplitude can of course still be defined, but since this amplitude is exponentially small in general (on account of the Gamow factor), mixing between left and right well states will be negligible unless the bottoms of the two wells are tuned to the same exponential sensitivity. The mathematical formulation of these points leads to extremely unpleasant transcendental equations, and the situation is not significantly improved in the case of symmetric potentials if one approaches the problem solely in terms of enforcing continuity of the wave function and its derivative. It is probably because of this fact that most introductory or intermediate quantum mechanics texts do not consider double-well tunnel splittings when they discuss the WKB method. Use of Herring's formula (with or without WKB) would make the problem much more tractable, and its widespread adoption is thus greatly to be desired.

APPENDIX B: WKB FORMULA FOR HIGHER STATE SPLITTINGS

It is to be expected that the formula given by Landau and Lifshitz [1] is increasingly accurate for higher pairs of states, assuming of course, that the WKB approximation is still applicable. We will find that this is indeed so. The splitting for the n th pair of levels, Δ_n , is given by

$$\Delta_n = g_n \frac{\hbar\omega}{\pi} \exp \left[- \int_{-a'_n}^{a'_n} \frac{|p|}{\hbar} dx \right], \quad (\text{B1})$$

where $\pm a'_n$ are the classical turning points for the n th energy level pair $(n + \frac{1}{2})\hbar\omega$, and

$$g_n = \frac{\sqrt{2\pi}}{n!} \left(n + \frac{1}{2} \right)^{n+\frac{1}{2}} e^{-(n+\frac{1}{2})}. \quad (\text{B2})$$

Note that if g_n were unity, we would have the formula of Ref. [1]. The corrections are indeed small: $g_0 = (\pi/e)^{1/2} \approx 1.075$, $g_1 \approx 1.028$, $g_2 \approx 1.017$, and so on. Stirling's formula for $n!$ shows that $g_n \rightarrow 1$ as $n \rightarrow \infty$.

The derivation of Eq. (B1) and the conditions under which it holds are straightforward though long. The starting point is still Herring's formula, Eq. (2.1). The procedure of Sec. II can be applied word for word, with a' , u_0 , and C_0 replaced by a'_n , u_n , and C_n , respectively.

The essential part is to find $\psi(x)$ in the classically forbidden region and match it onto the n th harmonic oscillator state in the vicinity of the well $x \approx a$. We leave it as an exercise — or see Ref. [19] — to show that the function $\Phi(x)$, defined in Eq. (2.7), is given in the overlap region by

$$\Phi(x) = -\frac{1}{2} \frac{m\omega}{\hbar} (a-x)^2 + \frac{2n+1}{2} \ln \left(\frac{2(a-x)}{u_n} \right) + \frac{2n+1}{4} + \dots, \quad (\text{B3})$$

so that the leading approximation to $\psi_0(x)$ is given by $C'_n(a-x)^n \exp(-x^2/2u_0)$, where

$$C'_n = \frac{C_n}{\omega^{1/2}} \left(\frac{2}{u_n} \right)^{n+\frac{1}{2}} \exp \left(\frac{1}{\hbar} \int_0^{a'_n} |p| dx + \frac{2n+1}{4} \right) \quad (\text{B4})$$

This is of the precise form required to be match on to the n th excited state harmonic oscillator wave function:

$$\psi_0(x) \approx \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \frac{2^{n/2}}{\sqrt{n!}} e^{-\xi^2/2} \left(\xi^n + O(\xi)^{n-2} \right), \quad (\text{B5})$$

with $\xi \equiv (a-x)/u_0$. The match yields the constant C_n , and the splitting Δ_n , which equals $2\hbar|C_n|^2$, is easily shown to be given by Eq. (B1) and (B2).

The calculation sketched above assumes that the turning point and the wavefunction in its vicinity are well approximated by taking the potential well to be parabolic. This is clearly less accurate as n gets large. Defining y and $U(y)$ as in Sec. IV, let us keep the cubic and quartic terms in y in $U(y)$:

$$U(y) = \frac{1}{2} m \omega^2 y^2 + \alpha y^3 + \beta y^4. \quad (\text{B6})$$

The wavefunction for the n th state can be found by perturbation theory assuming that α and β are small. The key requirement is that the correction terms be small compared to the unperturbed wavefunction near the turning point $y = u_n$. The dominant corrections are those that entail the Hermite polynomials of order $n+1$ through $n+4$. Since the coefficient of the largest power of x in these polynomials is known, the conditions for the corrections to be small are not difficult to find. They are

$$\alpha \ll \frac{6}{13n+11} (2n+1)^{-1/2} \left(\frac{m^3 \omega^5}{\hbar} \right)^{1/2}, \quad (\text{B7})$$

$$\beta \ll \frac{4}{(6n+7)(2n+1)} \frac{m^2 \omega^3}{\hbar}. \quad (\text{B8})$$

It is also possible to show that when these conditions hold, the corrections to u_n and the energies of the harmonic oscillator states are negligible, so that the conditions are self-consistently derived.

It need hardly be said that the conditions (B7) and (B8) are only necessary, not sufficient, for Eq. (B1) to apply. In addition, one must have the requirement for the WKB approximation itself to hold, which in the present context can be stated as $(n + \frac{1}{2})\hbar\omega \ll V(0) - V(a)$.

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